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Poly[[μ_4-naphthalene-1,4-dicarboxylato-$\kappa^4O:O':O'':O'''$-μ_2-naphthalene-1,4-dicarboxylato-$\kappa^4O,O':O'',O'''$-bis(2-phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene-κ^2N^7,N^8)-dimanganese(II)] *N*,*N*-dimethylformamide solvate]

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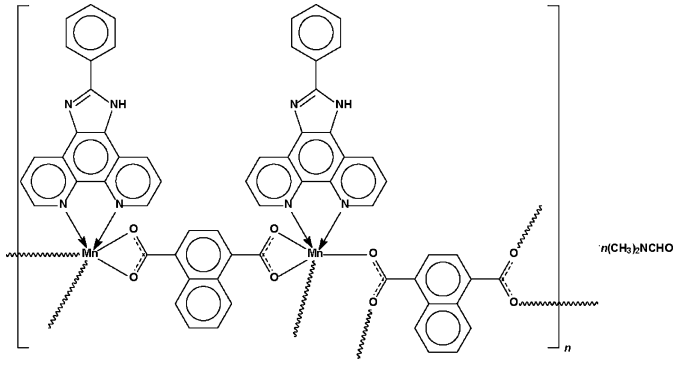
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.011 Å; disorder in main residue; R factor = 0.081; wR factor = 0.262; data-to-parameter ratio = 11.7.

One of the two 1,4-dicarboxylate dianions in the title compound, $[Mn_2(C_{12}H_6O_4)_2(C_{19}H_{12}N_4)_2]\cdot C_3H_7NO$, uses its two carboxylate groups to chelate two *N*-heterocycle-chelated Mn atoms; the other 1,4-dicarboxylate dianion binds to four such metal centers. The octahedrally coordinated Mn atoms are linked through the two dianions into a layer motif; the dimethylformamide molecules occupy the spaces between adjacent layers. Ten C atoms and attached H atoms of one dianion are disordered equally over two positions.

Related literature

There are several studies of 2-phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene-chelated metal compounds; for the structures of the manganese dicarboxylate adducts, see: Che (2006); Che & Liu (2006); Wang *et al.* (2006); Zhang *et al.* (2006).



Experimental

Crystal data

$[Mn_2(C_{12}H_6O_4)_2(C_{19}H_{12}N_4)_2]\cdot C_3H_7NO$
M_r = 1203.96
Triclinic, $P\overline{1}$
a = 9.240 (2) Å
b = 14.852 (5) Å
c = 21.921 (5) Å
α = 105.72 (1)°
β = 100.48 (1)°
γ = 101.67 (1)°
V = 2745.0 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.53 mm^{-1}
T = 295 (2) K
0.26 × 0.16 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.760, T_{max} = 0.940
21501 measured reflections
9443 independent reflections
4800 reflections with $I > 2\sigma(I)$
R_{int} = 0.084

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.262
S = 1.06
9443 reflections
810 parameters
158 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—O1^{i}	2.115 (5)	Mn2—O2	2.107 (5)
Mn1—O4^{ii}	2.105 (4)	Mn2—O3^{iii}	2.112 (5)
Mn1—O5	2.431 (5)	Mn2—O7	2.208 (5)
Mn1—O6	2.171 (5)	Mn2—O8	2.384 (5)
Mn1—N1	2.232 (5)	Mn2—N5	2.252 (6)
Mn1—N4	2.259 (5)	Mn2—N8	2.277 (5)

Symmetry codes: (i) $x, y+1, z$; (ii) $x+1, y+1, z$; (iii) $x+1, y, z$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001) and *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Base Construction Foundation of Jilin Normal University (No. 2006041), and the University of Malaya for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2195).

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supporting information

Acta Cryst. (2008). E**64**, m704–m705 [doi:10.1107/S1600536808010787]

Poly[[μ_4-naphthalene-1,4-dicarboxylato-κ^4O:O':O'':O'''-μ_2-naphthalene-1,4-dicarboxylato-κ^4O,O':O'',O'''-bis(2-phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene-κ^2N^7,N^8)dimanganese(II)] *N*,*N*-dimethylformamide solvate]

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S1. Comment

There are several studies of metal complexes of 2-phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene. Among these are several manganese complexes, the manganese succinate (Zhang *et al.*, 2006), manganese adipate (Wang *et al.*, 2006), manganese isophthalate (Che & Liu, 2006) and manganese terephthalate (Che, 2006) adducts, all of which feature carboxylate-bridged chain motifs. The title naphthalene-1,4-dicarboxylate adduct adopts a layer motif instead.

One of the two 1,4-dicarboxylate dianions in $Mn_2(C_{19}H_{12}N_4)_2(C_{12}H_6O_4)_2{\cdot}$DMF uses its two carboxyl $-CO_2$ groups to chelate to two *N*-heterocycle-chelated manganese atoms; the other 1,4-dicarboxylate dianion binds to four such metal centers. The octahedrally coordinated manganese atoms are linked through the two dianions into a layer motif; the DMF molecules occupy the spaces between adjacent layers.

S2. Experimental

Manganese dichloride dihydrate (0.1 mmol), naphthalene-1,4-dicarboxylic acid (0.1 mmol), 2-phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene (0.1 mmol), water (8 ml) and DMF (4 ml) were heated in a 23 ml, Teflon-lined, stainless-steel Parr bomb at 408 K for 2 days. Crystals were obtained in 40% yield.

S3. Refinement

The naphthalene-1,4-dicarboxylate dianion that is involved in μ_4-bridging is disordered over two positions in the fused-ring portion. This was refined as two rigid naphthalene groups of 1.39 Å sides; the occupancy was arbitrarily set as 0.5 as this could not be refined. The C1–C11 and C1′–C11 distances were restrained to within 0.01 Å of each other, as were the C4–C12 and C4′–C12 pair of distances. The anisotropic displacement factors of the two fused-rings were restrained to be nearly isotropic.

The carbon-bound H atoms were placed in calculated positions [C–H 0.93, N–H 0.86 Å and U_{iso}(H) 1.2U_{eq}(C,*N*)], and were included in the refinement in the riding-model approximation.

The final difference Fourier map had a large peak at 2.8 Å from O7, but this could not be modeled as a water molecule.

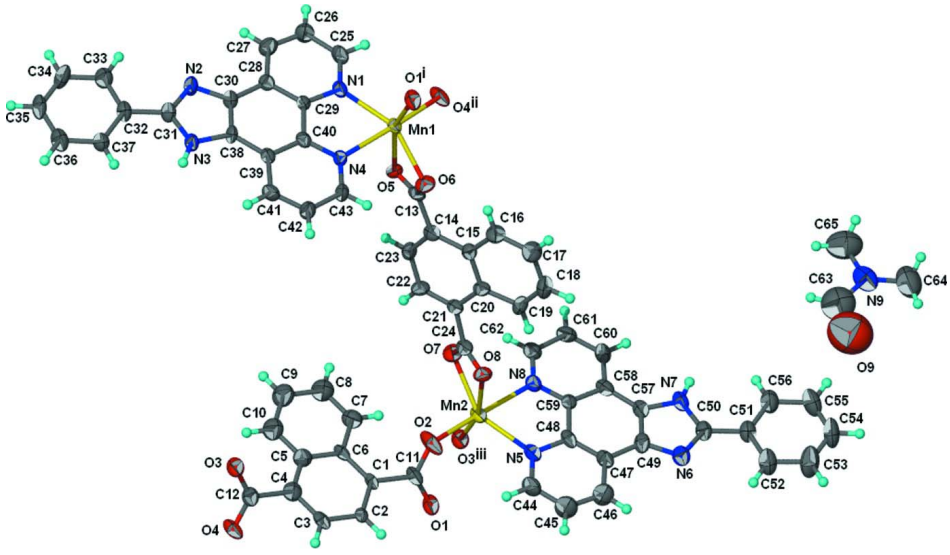

Figure 1

Thermal ellipsoid plot of $Mn_2(C_{19}H_{12}N_4)_2(C_{12}H_6O_4)_2\cdot$DMF; displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. The disorder in one of the naphthalene-1,4-dicarboxylate dianions is not shown. Symmetry codes are given in Table 1.

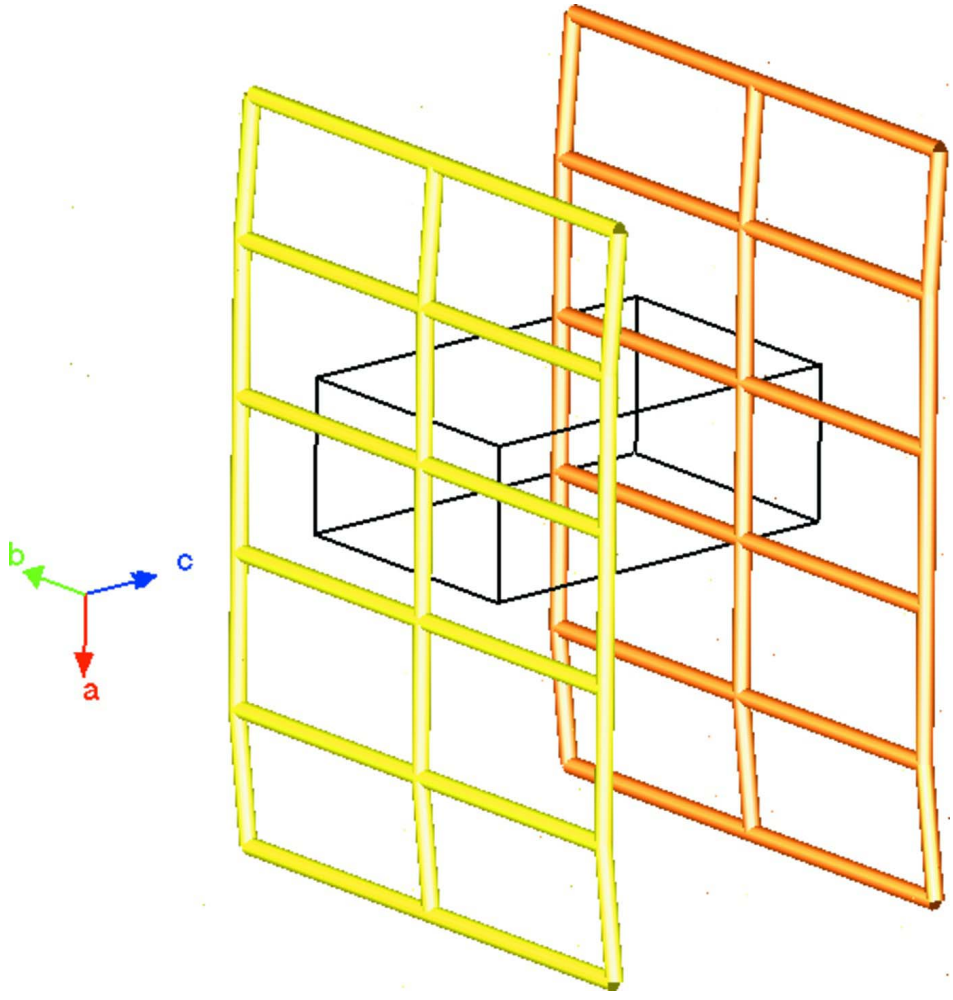

Figure 2

Layer structure of the manganese-naphthalene-1,4-dicarboxylate network as illustrated by *OLEX* (Dolomanov *et al.*, 2003).

Poly[[μ_4-naphthalene-1,4-dicarboxylato- $\kappa^4O:O':O'':O'''$- μ_2-naphthalene-1,4-dicarboxylato- $\kappa^4O,O':O'',O'''$-bis(2-phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene- κ^2N^7,N^8)dimanganese(II)] *N*,*N*-dimethylformamide solvate]

Crystal data

$[Mn_2(C_{12}H_6O_4)_2(C_{19}H_{12}N_4)_2]\cdot C_3H_7NO$
M_r = 1203.96
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.240 (2) Å
b = 14.852 (5) Å
c = 21.921 (5) Å
α = 105.72 (1)°
β = 100.48 (1)°
γ = 101.67 (1)°
V = 2745.0 (13) Å^3
Z = 2
$F(000)$ = 1236
D_x = 1.457 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 15789 reflections
θ = 3.0–27.5°
μ = 0.53 mm^{-1}
T = 295 K
Block, colorless
0.26 × 0.16 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.760, T_{max} = 0.940
21501 measured reflections
9443 independent reflections
4800 reflections with $I > 2\sigma(I)$
R_{int} = 0.084
θ_{max} = 25.0°, θ_{min} = 3.0°
h = −10→10
k = −17→17
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.262
S = 1.06
9443 reflections
810 parameters
158 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1308P)^2 + 1.0767P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Mn1	0.80675 (10)	0.75810 (7)	0.69248 (5)	0.0344 (3)	
Mn2	1.06512 (11)	0.08617 (8)	0.75021 (6)	0.0431 (3)	
O1	0.8244 (5)	−0.1078 (3)	0.7625 (2)	0.0484 (13)	
O2	0.8416 (5)	0.0418 (4)	0.7602 (3)	0.0721 (19)	
O3	0.0485 (5)	−0.0465 (4)	0.6792 (3)	0.0523 (14)	
O4	0.0263 (5)	−0.1993 (4)	0.6783 (3)	0.0539 (14)	
O5	0.8422 (5)	0.5979 (3)	0.6470 (2)	0.0394 (11)	
O6	0.8715 (5)	0.6725 (4)	0.7537 (2)	0.0464 (13)	
O7	1.0143 (5)	0.1880 (4)	0.6976 (3)	0.0500 (13)	
O8	1.0396 (5)	0.2427 (4)	0.8038 (2)	0.0445 (12)	
N1	0.6616 (5)	0.7650 (4)	0.6015 (3)	0.0358 (13)	
N2	0.1203 (6)	0.6871 (5)	0.4819 (3)	0.0418 (15)	
N3	0.0391 (6)	0.6310 (4)	0.5578 (3)	0.0372 (14)	
H3N	−0.0221	0.6062	0.5778	0.045*	
N4	0.5621 (6)	0.6932 (4)	0.6907 (3)	0.0335 (13)	
N5	1.2081 (6)	0.0765 (4)	0.8419 (3)	0.0433 (15)	
N6	1.7453 (6)	0.1593 (5)	0.9659 (3)	0.0479 (16)	
N7	1.8308 (6)	0.2076 (4)	0.8873 (3)	0.0439 (15)	
H7N	1.8936	0.2302	0.8671	0.053*	
N8	1.3130 (6)	0.1489 (4)	0.7526 (3)	0.0427 (15)	
C1	0.5938 (5)	−0.0627 (9)	0.7341 (5)	0.027 (8)	0.50
C2	0.5072 (7)	−0.1025 (11)	0.7707 (5)	0.029 (6)	0.50
H2	0.5551	−0.1156	0.8072	0.035*	0.50
C3	0.3489 (7)	−0.1228 (11)	0.7526 (5)	0.037 (5)	0.50
H3	0.2910	−0.1494	0.7771	0.045*	0.50

C4	0.2773 (5)	−0.1033 (10)	0.6980 (5)	0.048 (8)	0.50
C5	0.3640 (5)	−0.0635 (7)	0.6615 (4)	0.048 (10)	0.50
C6	0.5223 (5)	−0.0432 (7)	0.6795 (4)	0.034 (10)	0.50
C7	0.6089 (7)	−0.0034 (8)	0.6429 (5)	0.054 (4)	0.50
H7	0.7148	0.0102	0.6550	0.064*	0.50
C8	0.5373 (11)	0.0161 (8)	0.5883 (4)	0.071 (5)	0.50
H8	0.5953	0.0428	0.5639	0.085*	0.50
C9	0.3791 (11)	−0.0041 (8)	0.5703 (4)	0.067 (5)	0.50
H9	0.3312	0.0089	0.5338	0.081*	0.50
C10	0.2924 (8)	−0.0439 (9)	0.6069 (4)	0.063 (5)	0.50
H10	0.1865	−0.0575	0.5948	0.076*	0.50
C1′	0.5934 (5)	−0.0562 (9)	0.7394 (4)	0.047 (11)	0.50
C2′	0.5185 (7)	−0.0413 (10)	0.6835 (5)	0.048 (13)	0.50
H2′	0.5741	−0.0190	0.6567	0.058*	0.50
C3′	0.3604 (7)	−0.0597 (9)	0.6676 (4)	0.029 (8)	0.50
H3′	0.3102	−0.0497	0.6301	0.035*	0.50
C4′	0.2772 (5)	−0.0931 (8)	0.7076 (4)	0.021 (5)	0.50
C5′	0.3521 (5)	−0.1080 (5)	0.7635 (3)	0.028 (5)	0.50
C6′	0.5103 (5)	−0.0895 (6)	0.7794 (3)	0.040 (8)	0.50
C7′	0.5852 (6)	−0.1045 (7)	0.8353 (4)	0.039 (3)	0.50
H7′	0.6910	−0.0921	0.8460	0.047*	0.50
C8′	0.5020 (9)	−0.1378 (6)	0.8753 (3)	0.044 (4)	0.50
H8′	0.5522	−0.1478	0.9128	0.053*	0.50
C9′	0.3439 (9)	−0.1562 (6)	0.8594 (4)	0.046 (4)	0.50
H9′	0.2883	−0.1786	0.8862	0.055*	0.50
C10′	0.2690 (6)	−0.1413 (6)	0.8035 (4)	0.042 (3)	0.50
H10′	0.1632	−0.1537	0.7929	0.051*	0.50
C11	0.7665 (7)	−0.0412 (5)	0.7541 (4)	0.0456 (19)	
C12	0.1025 (8)	−0.1168 (6)	0.6854 (3)	0.0422 (18)	
C13	0.8782 (7)	0.6019 (5)	0.7074 (4)	0.0394 (17)	
C14	0.9218 (7)	0.5171 (5)	0.7226 (3)	0.0370 (16)	
C15	1.0253 (7)	0.5249 (5)	0.7819 (3)	0.0346 (16)	
C16	1.0953 (8)	0.6157 (5)	0.8332 (4)	0.0485 (19)	
H16	1.0697	0.6716	0.8290	0.058*	
C17	1.1988 (9)	0.6212 (6)	0.8881 (4)	0.056 (2)	
H17	1.2416	0.6804	0.9212	0.067*	
C18	1.2410 (9)	0.5380 (7)	0.8948 (4)	0.063 (2)	
H18	1.3150	0.5432	0.9315	0.075*	
C19	1.1752 (8)	0.4502 (6)	0.8485 (4)	0.0492 (19)	
H19	1.2030	0.3958	0.8545	0.059*	
C20	1.0646 (7)	0.4397 (5)	0.7909 (3)	0.0369 (16)	
C21	0.9922 (7)	0.3487 (5)	0.7412 (3)	0.0349 (16)	
C22	0.8966 (8)	0.3436 (5)	0.6850 (4)	0.0407 (17)	
H22	0.8517	0.2838	0.6527	0.049*	
C23	0.8646 (7)	0.4275 (5)	0.6751 (3)	0.0388 (17)	
H23	0.8027	0.4226	0.6352	0.047*	
C24	1.0185 (7)	0.2543 (5)	0.7487 (4)	0.0402 (17)	
C25	0.7115 (7)	0.8015 (5)	0.5574 (4)	0.0444 (18)	

H25	0.8161	0.8266	0.5646	0.053*
C26	0.6146 (8)	0.8038 (6)	0.5007 (4)	0.052 (2)
H26	0.6547	0.8283	0.4707	0.063*
C27	0.4607 (8)	0.7695 (6)	0.4904 (3)	0.0472 (19)
H27	0.3947	0.7705	0.4532	0.057*
C28	0.4023 (7)	0.7326 (5)	0.5366 (3)	0.0340 (15)
C29	0.5081 (7)	0.7313 (5)	0.5913 (3)	0.0304 (14)
C30	0.2444 (7)	0.6954 (5)	0.5310 (3)	0.0360 (16)
C31	−0.0010 (7)	0.6479 (5)	0.4995 (3)	0.0404 (17)
C32	−0.1577 (7)	0.6204 (5)	0.4597 (3)	0.0407 (17)
C33	−0.1849 (8)	0.6449 (6)	0.4017 (4)	0.054 (2)
H33	−0.1045	0.6802	0.3906	0.065*
C34	−0.3294 (9)	0.6169 (7)	0.3616 (4)	0.062 (2)
H34	−0.3451	0.6322	0.3229	0.074*
C35	−0.4512 (8)	0.5666 (6)	0.3772 (4)	0.057 (2)
H35	−0.5489	0.5482	0.3498	0.068*
C36	−0.4247 (8)	0.5435 (6)	0.4359 (4)	0.058 (2)
H36	−0.5062	0.5104	0.4477	0.070*
C37	−0.2806 (7)	0.5693 (6)	0.4757 (4)	0.0454 (18)
H37	−0.2649	0.5525	0.5138	0.055*
C38	0.1968 (6)	0.6614 (5)	0.5786 (3)	0.0330 (15)
C39	0.2984 (7)	0.6593 (5)	0.6347 (3)	0.0324 (15)
C40	0.4544 (7)	0.6934 (5)	0.6397 (3)	0.0344 (15)
C41	0.2561 (8)	0.6218 (5)	0.6840 (4)	0.0447 (18)
H41	0.1537	0.5966	0.6814	0.054*
C42	0.3656 (7)	0.6229 (6)	0.7346 (3)	0.0441 (18)
H42	0.3389	0.6003	0.7678	0.053*
C43	0.5183 (7)	0.6582 (5)	0.7367 (3)	0.0406 (17)
H43	0.5928	0.6574	0.7712	0.049*
C44	1.1542 (8)	0.0416 (6)	0.8854 (4)	0.059 (2)
H44	1.0494	0.0165	0.8777	0.070*
C45	1.2488 (10)	0.0416 (7)	0.9412 (4)	0.072 (3)
H45	1.2068	0.0186	0.9714	0.086*
C46	1.4035 (9)	0.0746 (7)	0.9535 (4)	0.064 (2)
H46	1.4675	0.0727	0.9909	0.076*
C47	1.4632 (7)	0.1115 (5)	0.9083 (4)	0.0427 (18)
C48	1.3611 (7)	0.1117 (5)	0.8531 (3)	0.0385 (17)
C49	1.6241 (7)	0.1468 (5)	0.9147 (4)	0.0435 (18)
C50	1.8678 (8)	0.1949 (5)	0.9482 (3)	0.0425 (18)
C51	2.0230 (8)	0.2242 (6)	0.9890 (4)	0.0481 (19)
C52	2.0480 (9)	0.2083 (7)	1.0480 (4)	0.067 (3)
H52	1.9674	0.1757	1.0606	0.081*
C53	2.1936 (11)	0.2406 (8)	1.0891 (4)	0.085 (3)
H53	2.2091	0.2319	1.1300	0.103*
C54	2.3144 (10)	0.2850 (8)	1.0708 (5)	0.079 (3)
H54	2.4119	0.3047	1.0985	0.095*
C55	2.2923 (9)	0.3005 (7)	1.0116 (5)	0.075 (3)
H55	2.3744	0.3301	0.9985	0.090*

C56	2.1443 (9)	0.2713 (7)	0.9708 (4)	0.063 (2)
H56	2.1278	0.2839	0.9311	0.075*
C57	1.6738 (7)	0.1767 (5)	0.8654 (3)	0.0386 (17)
C58	1.5753 (8)	0.1778 (5)	0.8082 (4)	0.0420 (17)
C59	1.4184 (7)	0.1474 (5)	0.8023 (3)	0.0336 (15)
C60	1.6205 (8)	0.2092 (6)	0.7593 (4)	0.055 (2)
H60	1.7237	0.2287	0.7609	0.066*
C61	1.5131 (9)	0.2115 (6)	0.7086 (4)	0.058 (2)
H61	1.5414	0.2336	0.6755	0.070*
C62	1.3589 (8)	0.1797 (6)	0.7075 (4)	0.053 (2)
H62	1.2856	0.1806	0.6726	0.064*
O9	2.5478 (19)	0.3811 (10)	0.9394 (7)	0.251 (7)
N9	2.6817 (9)	0.4487 (5)	0.8833 (4)	0.081 (2)
C63	2.5473 (15)	0.4057 (7)	0.8923 (7)	0.148 (6)
H63	2.4561	0.3956	0.8620	0.178*
C64	2.8345 (11)	0.4717 (9)	0.9235 (6)	0.120 (4)
H64A	2.8304	0.4595	0.9641	0.181*
H64B	2.8841	0.5388	0.9322	0.181*
H64C	2.8908	0.4320	0.9010	0.181*
C65	2.6539 (17)	0.4727 (9)	0.8232 (5)	0.136 (5)
H65A	2.5459	0.4589	0.8055	0.204*
H65B	2.6969	0.4346	0.7921	0.204*
H65C	2.7004	0.5404	0.8321	0.204*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0223 (5)	0.0271 (6)	0.0533 (7)	0.0068 (4)	0.0067 (5)	0.0140 (5)
Mn2	0.0265 (6)	0.0289 (7)	0.0766 (8)	0.0103 (5)	0.0118 (5)	0.0196 (6)
O1	0.033 (3)	0.033 (3)	0.070 (3)	0.012 (2)	0.003 (2)	0.006 (3)
O2	0.029 (3)	0.034 (3)	0.151 (6)	0.009 (3)	0.035 (3)	0.016 (4)
O3	0.035 (3)	0.038 (3)	0.083 (4)	0.016 (2)	0.008 (3)	0.019 (3)
O4	0.029 (3)	0.031 (3)	0.101 (4)	0.007 (2)	0.025 (3)	0.016 (3)
O5	0.037 (3)	0.040 (3)	0.046 (3)	0.011 (2)	0.008 (2)	0.024 (2)
O6	0.051 (3)	0.040 (3)	0.059 (3)	0.025 (3)	0.017 (3)	0.020 (3)
O7	0.052 (3)	0.033 (3)	0.066 (3)	0.020 (3)	0.009 (3)	0.016 (3)
O8	0.042 (3)	0.042 (3)	0.063 (3)	0.018 (2)	0.016 (3)	0.030 (3)
N1	0.026 (3)	0.035 (4)	0.044 (3)	0.005 (2)	0.009 (3)	0.012 (3)
N2	0.027 (3)	0.060 (4)	0.037 (3)	0.008 (3)	0.004 (3)	0.018 (3)
N3	0.023 (3)	0.048 (4)	0.040 (3)	0.007 (3)	0.007 (3)	0.017 (3)
N4	0.029 (3)	0.027 (3)	0.038 (3)	0.005 (2)	0.000 (3)	0.008 (3)
N5	0.032 (3)	0.031 (4)	0.066 (4)	0.006 (3)	0.013 (3)	0.014 (3)
N6	0.040 (3)	0.051 (4)	0.053 (4)	0.013 (3)	0.013 (3)	0.014 (3)
N7	0.030 (3)	0.038 (4)	0.058 (4)	0.006 (3)	0.010 (3)	0.007 (3)
N8	0.028 (3)	0.038 (4)	0.065 (4)	0.009 (3)	0.011 (3)	0.021 (3)
C1	0.015 (10)	0.023 (10)	0.042 (10)	0.006 (7)	0.014 (7)	0.003 (6)
C2	0.026 (8)	0.017 (7)	0.036 (8)	0.004 (6)	0.000 (6)	0.002 (6)
C3	0.034 (9)	0.019 (7)	0.049 (8)	0.001 (6)	0.013 (7)	−0.003 (6)

C4	0.050 (11)	0.036 (11)	0.053 (9)	0.012 (8)	0.008 (8)	0.008 (7)
C5	0.045 (13)	0.047 (13)	0.055 (12)	0.013 (8)	0.013 (9)	0.020 (8)
C6	0.023 (12)	0.030 (13)	0.048 (12)	0.002 (7)	0.018 (8)	0.011 (7)
C7	0.053 (7)	0.049 (8)	0.061 (8)	0.011 (6)	0.018 (6)	0.021 (6)
C8	0.068 (8)	0.076 (9)	0.073 (8)	0.016 (7)	0.018 (7)	0.032 (7)
C9	0.059 (8)	0.076 (9)	0.075 (8)	0.027 (7)	0.019 (7)	0.030 (7)
C10	0.054 (8)	0.070 (9)	0.069 (8)	0.019 (7)	0.015 (7)	0.026 (7)
C1′	0.038 (13)	0.035 (13)	0.060 (13)	0.010 (9)	0.008 (9)	0.004 (8)
C2′	0.039 (15)	0.043 (15)	0.061 (14)	0.011 (9)	0.016 (9)	0.011 (8)
C3′	0.015 (9)	0.029 (10)	0.044 (10)	0.015 (7)	0.005 (7)	0.009 (6)
C4′	0.010 (7)	0.008 (7)	0.045 (8)	0.005 (5)	0.013 (6)	0.003 (5)
C5′	0.025 (8)	0.016 (8)	0.040 (8)	0.010 (6)	0.007 (6)	0.001 (6)
C6′	0.043 (10)	0.034 (10)	0.047 (10)	0.013 (7)	0.017 (8)	0.011 (7)
C7′	0.038 (6)	0.034 (7)	0.045 (7)	0.015 (5)	0.006 (5)	0.009 (5)
C8′	0.041 (6)	0.042 (7)	0.051 (7)	0.015 (6)	0.010 (6)	0.015 (6)
C9′	0.054 (7)	0.035 (7)	0.053 (7)	0.009 (6)	0.026 (6)	0.014 (6)
C10′	0.037 (6)	0.036 (7)	0.054 (7)	0.013 (5)	0.017 (6)	0.008 (6)
C11	0.026 (3)	0.029 (4)	0.075 (5)	0.004 (3)	0.012 (4)	0.009 (4)
C12	0.035 (4)	0.043 (5)	0.047 (4)	0.012 (4)	0.011 (3)	0.010 (4)
C13	0.028 (3)	0.036 (4)	0.063 (5)	0.008 (3)	0.019 (4)	0.024 (4)
C14	0.032 (4)	0.032 (4)	0.052 (4)	0.013 (3)	0.016 (3)	0.014 (3)
C15	0.028 (3)	0.040 (4)	0.040 (4)	0.010 (3)	0.011 (3)	0.015 (3)
C16	0.052 (5)	0.033 (5)	0.059 (5)	0.017 (4)	0.009 (4)	0.011 (4)
C17	0.062 (5)	0.042 (5)	0.052 (5)	0.014 (4)	0.004 (4)	0.004 (4)
C18	0.045 (5)	0.070 (7)	0.061 (5)	0.010 (5)	−0.008 (4)	0.020 (5)
C19	0.041 (4)	0.047 (5)	0.057 (5)	0.015 (4)	−0.004 (4)	0.021 (4)
C20	0.033 (3)	0.035 (4)	0.053 (4)	0.014 (3)	0.017 (3)	0.022 (4)
C21	0.030 (3)	0.030 (4)	0.048 (4)	0.009 (3)	0.013 (3)	0.015 (3)
C22	0.047 (4)	0.028 (4)	0.052 (4)	0.016 (3)	0.013 (4)	0.017 (3)
C23	0.029 (3)	0.050 (5)	0.040 (4)	0.012 (3)	0.008 (3)	0.018 (4)
C24	0.029 (4)	0.033 (4)	0.065 (5)	0.015 (3)	0.014 (4)	0.021 (4)
C25	0.027 (3)	0.050 (5)	0.060 (5)	0.008 (3)	0.019 (4)	0.019 (4)
C26	0.047 (4)	0.063 (6)	0.050 (5)	0.011 (4)	0.015 (4)	0.025 (4)
C27	0.049 (4)	0.060 (6)	0.039 (4)	0.018 (4)	0.013 (4)	0.023 (4)
C28	0.031 (3)	0.034 (4)	0.038 (4)	0.009 (3)	0.012 (3)	0.011 (3)
C29	0.025 (3)	0.028 (4)	0.036 (4)	0.004 (3)	0.005 (3)	0.011 (3)
C30	0.030 (4)	0.041 (4)	0.033 (4)	0.009 (3)	0.007 (3)	0.008 (3)
C31	0.029 (4)	0.048 (5)	0.041 (4)	0.013 (3)	0.008 (3)	0.010 (4)
C32	0.030 (4)	0.044 (5)	0.040 (4)	0.010 (3)	0.005 (3)	0.003 (3)
C33	0.042 (4)	0.064 (6)	0.057 (5)	0.011 (4)	0.011 (4)	0.023 (4)
C34	0.045 (5)	0.088 (7)	0.057 (5)	0.029 (5)	−0.001 (4)	0.030 (5)
C35	0.027 (4)	0.065 (6)	0.067 (5)	0.016 (4)	−0.001 (4)	0.010 (5)
C36	0.037 (4)	0.060 (6)	0.069 (6)	0.007 (4)	0.009 (4)	0.013 (5)
C37	0.034 (4)	0.049 (5)	0.052 (4)	0.009 (3)	0.007 (4)	0.019 (4)
C38	0.020 (3)	0.042 (4)	0.036 (4)	0.011 (3)	0.002 (3)	0.011 (3)
C39	0.026 (3)	0.027 (4)	0.043 (4)	0.007 (3)	0.007 (3)	0.009 (3)
C40	0.034 (4)	0.023 (4)	0.039 (4)	0.003 (3)	0.005 (3)	0.003 (3)
C41	0.033 (4)	0.048 (5)	0.060 (5)	0.007 (3)	0.019 (4)	0.026 (4)

C42	0.036 (4)	0.060 (5)	0.040 (4)	0.009 (4)	0.008 (3)	0.024 (4)
C43	0.027 (3)	0.051 (5)	0.042 (4)	0.007 (3)	0.002 (3)	0.019 (4)
C44	0.033 (4)	0.066 (6)	0.085 (6)	0.009 (4)	0.021 (5)	0.037 (5)
C45	0.056 (5)	0.102 (8)	0.075 (6)	0.018 (5)	0.032 (5)	0.049 (6)
C46	0.056 (5)	0.084 (7)	0.062 (5)	0.020 (5)	0.021 (5)	0.033 (5)
C47	0.032 (4)	0.041 (5)	0.056 (5)	0.007 (3)	0.017 (4)	0.015 (4)
C48	0.029 (3)	0.024 (4)	0.054 (4)	0.003 (3)	0.011 (3)	0.001 (3)
C49	0.033 (4)	0.042 (5)	0.051 (4)	0.016 (3)	0.005 (4)	0.007 (4)
C50	0.034 (4)	0.045 (5)	0.045 (4)	0.011 (3)	0.009 (3)	0.009 (4)
C51	0.038 (4)	0.053 (5)	0.045 (4)	0.012 (4)	0.006 (4)	0.006 (4)
C52	0.042 (5)	0.090 (8)	0.057 (5)	0.010 (5)	0.008 (4)	0.013 (5)
C53	0.066 (6)	0.131 (10)	0.034 (5)	0.015 (6)	−0.004 (5)	0.006 (5)
C54	0.037 (5)	0.105 (9)	0.070 (7)	0.008 (5)	−0.006 (5)	0.010 (6)
C55	0.039 (5)	0.084 (8)	0.084 (7)	0.002 (5)	0.013 (5)	0.011 (6)
C56	0.046 (5)	0.064 (6)	0.067 (6)	0.010 (4)	0.002 (4)	0.015 (5)
C57	0.030 (4)	0.031 (4)	0.053 (4)	0.012 (3)	0.012 (4)	0.008 (3)
C58	0.037 (4)	0.034 (4)	0.057 (5)	0.006 (3)	0.017 (4)	0.015 (4)
C59	0.032 (3)	0.023 (4)	0.044 (4)	0.008 (3)	0.006 (3)	0.009 (3)
C60	0.026 (4)	0.063 (6)	0.078 (6)	0.008 (4)	0.010 (4)	0.031 (5)
C61	0.047 (5)	0.056 (6)	0.082 (6)	0.007 (4)	0.019 (5)	0.041 (5)
C62	0.038 (4)	0.050 (5)	0.077 (6)	0.007 (4)	0.015 (4)	0.032 (5)
O9	0.266 (11)	0.249 (11)	0.242 (10)	0.055 (8)	0.089 (8)	0.080 (8)
N9	0.072 (5)	0.072 (5)	0.096 (5)	0.011 (4)	0.031 (4)	0.019 (4)
C63	0.159 (8)	0.143 (8)	0.145 (8)	0.046 (6)	0.043 (6)	0.044 (6)
C64	0.086 (9)	0.110 (11)	0.142 (11)	0.010 (8)	0.012 (8)	0.027 (9)
C65	0.180 (9)	0.124 (9)	0.122 (8)	0.042 (7)	0.061 (7)	0.052 (7)

Geometric parameters (Å, º)

Mn1—O1^{i}	2.115 (5)	C17—C18	1.406 (11)
Mn1—O4^{ii}	2.105 (4)	C17—H17	0.9300
Mn1—O5	2.431 (5)	C18—C19	1.355 (11)
Mn1—O6	2.171 (5)	C18—H18	0.9300
Mn1—N1	2.232 (5)	C19—C20	1.421 (9)
Mn1—N4	2.259 (5)	C19—H19	0.9300
Mn2—O2	2.107 (5)	C20—C21	1.426 (9)
Mn2—O3^{iii}	2.112 (5)	C21—C22	1.351 (9)
Mn2—O7	2.208 (5)	C21—C24	1.516 (9)
Mn2—O8	2.384 (5)	C22—C23	1.400 (9)
Mn2—N5	2.252 (6)	C22—H22	0.9300
Mn2—N8	2.277 (5)	C23—H23	0.9300
O1—C11	1.255 (8)	C25—C26	1.407 (10)
O2—C11	1.246 (8)	C25—H25	0.9300
O3—C12	1.272 (8)	C26—C27	1.363 (9)
O4—C12	1.237 (8)	C26—H26	0.9300
O4—Mn1^{iv}	2.105 (4)	C27—C28	1.414 (9)
O5—C13	1.285 (8)	C27—H27	0.9300
O6—C13	1.268 (8)	C28—C29	1.410 (9)

O7—C24	1.264 (8)	C28—C30	1.421 (8)
O8—C24	1.252 (8)	C29—C40	1.445 (9)
N1—C25	1.335 (8)	C30—C38	1.378 (9)
N1—C29	1.360 (7)	C31—C32	1.460 (9)
N2—C31	1.325 (8)	C32—C37	1.389 (9)
N2—C30	1.381 (8)	C32—C33	1.408 (10)
N3—C31	1.370 (9)	C33—C34	1.371 (10)
N3—C38	1.384 (7)	C33—H33	0.9300
N3—H3N	0.8600	C34—C35	1.371 (11)
N4—C43	1.342 (8)	C34—H34	0.9300
N4—C40	1.357 (8)	C35—C36	1.411 (11)
N5—C44	1.327 (9)	C35—H35	0.9300
N5—C48	1.356 (8)	C36—C37	1.367 (10)
N6—C50	1.319 (8)	C36—H36	0.9300
N6—C49	1.375 (9)	C37—H37	0.9300
N7—C57	1.380 (8)	C38—C39	1.416 (9)
N7—C50	1.390 (9)	C39—C40	1.401 (8)
N7—H7N	0.8600	C39—C41	1.423 (9)
N8—C62	1.298 (9)	C41—C42	1.353 (9)
N8—C59	1.331 (8)	C41—H41	0.9300
C1—C2	1.3900	C42—C43	1.390 (9)
C1—C6	1.3900	C42—H42	0.9300
C1—C11	1.517 (8)	C43—H43	0.9300
C2—C3	1.3900	C44—C45	1.370 (11)
C2—H2	0.9300	C44—H44	0.9300
C3—C4	1.3900	C45—C46	1.365 (11)
C3—H3	0.9300	C45—H45	0.9300
C4—C5	1.3900	C46—C47	1.399 (10)
C4—C12	1.550 (8)	C46—H46	0.9300
C5—C6	1.3900	C47—C48	1.393 (10)
C5—C10	1.3900	C47—C49	1.441 (9)
C6—C7	1.3900	C48—C59	1.490 (9)
C7—C8	1.3900	C49—C57	1.391 (10)
C7—H7	0.9300	C50—C51	1.454 (10)
C8—C9	1.3900	C51—C52	1.365 (11)
C8—H8	0.9300	C51—C56	1.379 (11)
C9—C10	1.3900	C52—C53	1.384 (11)
C9—H9	0.9300	C52—H52	0.9300
C10—H10	0.9300	C53—C54	1.360 (13)
C1′—C2′	1.3900	C53—H53	0.9300
C1′—C6′	1.3900	C54—C55	1.365 (13)
C1′—C11	1.530 (8)	C54—H54	0.9300
C2′—C3′	1.3900	C55—C56	1.400 (11)
C2′—H2′	0.9300	C55—H55	0.9300
C3′—C4′	1.3900	C56—H56	0.9300
C3′—H3′	0.9300	C57—C58	1.415 (10)
C4′—C5′	1.3900	C58—C60	1.377 (10)
C4′—C12	1.535 (8)	C58—C59	1.399 (9)

C5′—C6′	1.3900	C60—C61	1.362 (11)
C5′—C10′	1.3900	C60—H60	0.9300
C6′—C7′	1.3900	C61—C62	1.401 (10)
C7′—C8′	1.3900	C61—H61	0.9300
C7′—H7′	0.9300	C62—H62	0.9300
C8′—C9′	1.3900	O9—C63	1.18 (2)
C8′—H8′	0.9300	N9—C63	1.351 (9)
C9′—C10′	1.3900	N9—C64	1.440 (8)
C9′—H9′	0.9300	N9—C65	1.449 (8)
C10′—H10′	0.9300	C63—H63	0.9300
C13—C14	1.499 (9)	C64—H64A	0.9600
C14—C23	1.378 (9)	C64—H64B	0.9600
C14—C15	1.427 (9)	C64—H64C	0.9600
C15—C16	1.437 (10)	C65—H65A	0.9600
C15—C20	1.438 (9)	C65—H65B	0.9600
C16—C17	1.366 (10)	C65—H65C	0.9600
C16—H16	0.9300		

O4^{ii}—Mn1—O1^{i}	94.88 (19)	C20—C19—H19	119.3
O4^{ii}—Mn1—O6	94.6 (2)	C19—C20—C21	123.1 (6)
O1^{i}—Mn1—O6	102.2 (2)	C19—C20—C15	118.5 (7)
O4^{ii}—Mn1—N1	101.0 (2)	C21—C20—C15	118.3 (6)
O1^{i}—Mn1—N1	103.1 (2)	C22—C21—C20	120.8 (6)
O6—Mn1—N1	148.9 (2)	C22—C21—C24	117.3 (7)
O4^{ii}—Mn1—N4	170.2 (2)	C20—C21—C24	121.9 (6)
O1^{i}—Mn1—N4	94.20 (18)	C21—C22—C23	120.6 (7)
O6—Mn1—N4	87.09 (19)	C21—C22—H22	119.7
N1—Mn1—N4	73.34 (19)	C23—C22—H22	119.7
O4^{ii}—Mn1—O5	81.46 (17)	C14—C23—C22	122.0 (7)
O1^{i}—Mn1—O5	159.11 (18)	C14—C23—H23	119.0
O6—Mn1—O5	57.90 (17)	C22—C23—H23	119.0
N1—Mn1—O5	97.75 (18)	O8—C24—O7	121.9 (6)
N4—Mn1—O5	91.31 (17)	O8—C24—C21	120.3 (7)
O2—Mn2—O3^{iii}	94.0 (2)	O7—C24—C21	117.8 (7)
O2—Mn2—O7	95.2 (2)	O8—C24—Mn2	65.0 (4)
O3^{iii}—Mn2—O7	107.4 (2)	O7—C24—Mn2	56.9 (4)
O2—Mn2—N5	102.3 (2)	C21—C24—Mn2	174.7 (5)
O3^{iii}—Mn2—N5	103.1 (2)	N1—C25—C26	123.6 (6)
O7—Mn2—N5	143.5 (2)	N1—C25—H25	118.2
O2—Mn2—N8	172.5 (2)	C26—C25—H25	118.2
O3^{iii}—Mn2—N8	93.1 (2)	C27—C26—C25	118.9 (7)
O7—Mn2—N8	85.2 (2)	C27—C26—H26	120.6
N5—Mn2—N8	73.5 (2)	C25—C26—H26	120.6
O2—Mn2—O8	82.28 (18)	C26—C27—C28	119.6 (7)
O3^{iii}—Mn2—O8	163.32 (19)	C26—C27—H27	120.2
O7—Mn2—O8	57.07 (18)	C28—C27—H27	120.2
N5—Mn2—O8	93.55 (19)	C29—C28—C27	117.6 (6)
N8—Mn2—O8	91.70 (19)	C29—C28—C30	118.0 (6)

C11—O1—Mn1^{v}	127.7 (5)	C27—C28—C30	124.3 (6)
C11—O2—Mn2	128.6 (5)	N1—C29—C28	122.9 (6)
C12—O3—Mn2^{vi}	129.6 (5)	N1—C29—C40	117.3 (6)
C12—O4—Mn1^{iv}	128.5 (4)	C28—C29—C40	119.8 (5)
C13—O5—Mn1	83.7 (4)	C38—C30—N2	110.4 (5)
C13—O6—Mn1	95.8 (4)	C38—C30—C28	120.7 (6)
C24—O7—Mn2	94.4 (4)	N2—C30—C28	128.9 (6)
C24—O8—Mn2	86.6 (4)	N2—C31—N3	111.7 (6)
C25—N1—C29	117.5 (6)	N2—C31—C32	124.3 (6)
C25—N1—Mn1	126.0 (4)	N3—C31—C32	123.8 (6)
C29—N1—Mn1	116.5 (4)	C37—C32—C33	118.5 (6)
C31—N2—C30	105.4 (5)	C37—C32—C31	123.1 (7)
C31—N3—C38	107.0 (5)	C33—C32—C31	118.5 (6)
C31—N3—H3N	126.5	C34—C33—C32	120.4 (7)
C38—N3—H3N	126.5	C34—C33—H33	119.8
C43—N4—C40	119.2 (5)	C32—C33—H33	119.8
C43—N4—Mn1	124.8 (4)	C33—C34—C35	121.3 (8)
C40—N4—Mn1	115.9 (4)	C33—C34—H34	119.3
C44—N5—C48	118.7 (7)	C35—C34—H34	119.3
C44—N5—Mn2	125.3 (5)	C34—C35—C36	118.4 (7)
C48—N5—Mn2	116.0 (5)	C34—C35—H35	120.8
C50—N6—C49	105.2 (6)	C36—C35—H35	120.8
C57—N7—C50	106.7 (6)	C37—C36—C35	120.8 (7)
C57—N7—H7N	126.7	C37—C36—H36	119.6
C50—N7—H7N	126.7	C35—C36—H36	119.6
C62—N8—C59	118.0 (6)	C36—C37—C32	120.6 (7)
C62—N8—Mn2	125.3 (5)	C36—C37—H37	119.7
C59—N8—Mn2	116.5 (4)	C32—C37—H37	119.7
C2—C1—C6	120.0	C30—C38—N3	105.5 (5)
C2—C1—C11	119.5 (5)	C30—C38—C39	123.4 (6)
C6—C1—C11	120.5 (5)	N3—C38—C39	131.0 (6)
C1—C2—C3	120.0	C40—C39—C38	116.2 (6)
C1—C2—H2	120.0	C40—C39—C41	117.8 (6)
C3—C2—H2	120.0	C38—C39—C41	125.9 (6)
C4—C3—C2	120.0	N4—C40—C39	121.4 (6)
C4—C3—H3	120.0	N4—C40—C29	116.9 (5)
C2—C3—H3	120.0	C39—C40—C29	121.8 (6)
C3—C4—C5	120.0	C42—C41—C39	119.7 (6)
C3—C4—C12	117.1 (5)	C42—C41—H41	120.1
C5—C4—C12	122.6 (5)	C39—C41—H41	120.1
C6—C5—C4	120.0	C41—C42—C43	119.4 (6)
C6—C5—C10	120.0	C41—C42—H42	120.3
C4—C5—C10	120.0	C43—C42—H42	120.3
C7—C6—C5	120.0	N4—C43—C42	122.4 (6)
C7—C6—C1	120.0	N4—C43—H43	118.8
C5—C6—C1	120.0	C42—C43—H43	118.8
C6—C7—C8	120.0	N5—C44—C45	121.8 (7)
C6—C7—H7	120.0	N5—C44—H44	119.1

C8—C7—H7	120.0	C45—C44—H44	119.1
C9—C8—C7	120.0	C46—C45—C44	121.2 (8)
C9—C8—H8	120.0	C46—C45—H45	119.4
C7—C8—H8	120.0	C44—C45—H45	119.4
C8—C9—C10	120.0	C45—C46—C47	118.1 (8)
C8—C9—H9	120.0	C45—C46—H46	120.9
C10—C9—H9	120.0	C47—C46—H46	120.9
C9—C10—C5	120.0	C48—C47—C46	118.1 (7)
C9—C10—H10	120.0	C48—C47—C49	118.2 (6)
C5—C10—H10	120.0	C46—C47—C49	123.7 (7)
C2′—C1′—C6′	120.0	N5—C48—C47	122.1 (6)
C2′—C1′—C11	119.4 (5)	N5—C48—C59	117.4 (6)
C6′—C1′—C11	120.6 (5)	C47—C48—C59	120.4 (6)
C1′—C2′—C3′	120.0	N6—C49—C57	111.1 (6)
C1′—C2′—H2′	120.0	N6—C49—C47	129.0 (7)
C3′—C2′—H2′	120.0	C57—C49—C47	119.9 (6)
C2′—C3′—C4′	120.0	N6—C50—N7	111.9 (6)
C2′—C3′—H3′	120.0	N6—C50—C51	124.6 (7)
C4′—C3′—H3′	120.0	N7—C50—C51	123.3 (6)
C5′—C4′—C3′	120.0	C52—C51—C56	119.3 (7)
C5′—C4′—C12	122.6 (4)	C52—C51—C50	119.0 (7)
C3′—C4′—C12	117.4 (4)	C56—C51—C50	121.7 (7)
C4′—C5′—C6′	120.0	C51—C52—C53	119.8 (8)
C4′—C5′—C10′	120.0	C51—C52—H52	120.1
C6′—C5′—C10′	120.0	C53—C52—H52	120.1
C7′—C6′—C5′	120.0	C54—C53—C52	121.2 (9)
C7′—C6′—C1′	120.0	C54—C53—H53	119.4
C5′—C6′—C1′	120.0	C52—C53—H53	119.4
C8′—C7′—C6′	120.0	C53—C54—C55	119.9 (8)
C8′—C7′—H7′	120.0	C53—C54—H54	120.0
C6′—C7′—H7′	120.0	C55—C54—H54	120.0
C9′—C8′—C7′	120.0	C54—C55—C56	119.2 (8)
C9′—C8′—H8′	120.0	C54—C55—H55	120.4
C7′—C8′—H8′	120.0	C56—C55—H55	120.4
C10′—C9′—C8′	120.0	C51—C56—C55	120.5 (9)
C10′—C9′—H9′	120.0	C51—C56—H56	119.7
C8′—C9′—H9′	120.0	C55—C56—H56	119.7
C9′—C10′—C5′	120.0	N7—C57—C49	105.1 (6)
C9′—C10′—H10′	120.0	N7—C57—C58	130.6 (7)
C5′—C10′—H10′	120.0	C49—C57—C58	124.2 (6)
O2—C11—O1	124.3 (6)	C60—C58—C59	117.5 (7)
O2—C11—C1	117.2 (7)	C60—C58—C57	125.7 (6)
O1—C11—C1	118.5 (7)	C59—C58—C57	116.8 (6)
O2—C11—C1′	114.9 (7)	N8—C59—C58	123.1 (6)
O1—C11—C1′	120.7 (7)	N8—C59—C48	116.4 (6)
O4—C12—O3	125.5 (6)	C58—C59—C48	120.4 (6)
O4—C12—C4′	118.6 (7)	C61—C60—C58	119.6 (7)
O3—C12—C4′	115.8 (7)	C61—C60—H60	120.2

O4—C12—C4	115.2 (7)	C58—C60—H60	120.2
O3—C12—C4	119.2 (8)	C60—C61—C62	118.2 (7)
O6—C13—O5	122.5 (6)	C60—C61—H61	120.9
O6—C13—C14	119.2 (6)	C62—C61—H61	120.9
O5—C13—C14	118.2 (6)	N8—C62—C61	123.5 (8)
O6—C13—Mn1	55.5 (3)	N8—C62—H62	118.2
O5—C13—Mn1	67.1 (4)	C61—C62—H62	118.2
C14—C13—Mn1	174.6 (5)	C63—N9—C64	129.9 (11)
C23—C14—C15	118.5 (6)	C63—N9—C65	109.3 (11)
C23—C14—C13	117.7 (7)	C64—N9—C65	120.8 (10)
C15—C14—C13	123.7 (7)	O9—C63—N9	118.8 (16)
C14—C15—C16	122.5 (6)	O9—C63—H63	120.6
C14—C15—C20	119.6 (6)	N9—C63—H63	120.6
C16—C15—C20	117.9 (6)	N9—C64—H64A	109.5
C17—C16—C15	120.9 (7)	N9—C64—H64B	109.5
C17—C16—H16	119.6	H64A—C64—H64B	109.5
C15—C16—H16	119.6	N9—C64—H64C	109.5
C16—C17—C18	120.4 (8)	H64A—C64—H64C	109.5
C16—C17—H17	119.8	H64B—C64—H64C	109.5
C18—C17—H17	119.8	N9—C65—H65A	109.5
C19—C18—C17	120.8 (8)	N9—C65—H65B	109.5
C19—C18—H18	119.6	H65A—C65—H65B	109.5
C17—C18—H18	119.6	N9—C65—H65C	109.5
C18—C19—C20	121.3 (7)	H65A—C65—H65C	109.5
C18—C19—H19	119.3	H65B—C65—H65C	109.5

O3^{iii}—Mn2—O2—C11	31.4 (8)	C13—C14—C15—C16	1.2 (9)
O7—Mn2—O2—C11	139.3 (8)	C23—C14—C15—C20	−1.1 (9)
N5—Mn2—O2—C11	−73.0 (8)	C13—C14—C15—C20	−177.6 (5)
O8—Mn2—O2—C11	−165.0 (8)	C14—C15—C16—C17	−177.1 (7)
C24—Mn2—O2—C11	167.4 (8)	C20—C15—C16—C17	1.6 (10)
O4^{ii}—Mn1—O5—C13	98.9 (4)	C15—C16—C17—C18	1.2 (12)
O1^{i}—Mn1—O5—C13	17.7 (6)	C16—C17—C18—C19	−2.9 (13)
O6—Mn1—O5—C13	−1.9 (3)	C17—C18—C19—C20	1.6 (12)
N1—Mn1—O5—C13	−161.1 (3)	C18—C19—C20—C21	−179.7 (7)
N4—Mn1—O5—C13	−87.7 (4)	C18—C19—C20—C15	1.2 (10)
O4^{ii}—Mn1—O6—C13	−75.0 (4)	C14—C15—C20—C19	176.1 (6)
O1^{i}—Mn1—O6—C13	−171.0 (4)	C16—C15—C20—C19	−2.7 (9)
N1—Mn1—O6—C13	45.1 (5)	C14—C15—C20—C21	−3.1 (8)
N4—Mn1—O6—C13	95.4 (4)	C16—C15—C20—C21	178.1 (6)
O5—Mn1—O6—C13	2.0 (3)	C19—C20—C21—C22	−174.9 (6)
O2—Mn2—O7—C24	78.8 (4)	C15—C20—C21—C22	4.3 (9)
O3^{iii}—Mn2—O7—C24	174.7 (4)	C19—C20—C21—C24	5.1 (9)
N5—Mn2—O7—C24	−39.9 (5)	C15—C20—C21—C24	−175.8 (5)
N8—Mn2—O7—C24	−93.6 (4)	C20—C21—C22—C23	−1.1 (9)
O8—Mn2—O7—C24	1.5 (4)	C24—C21—C22—C23	178.9 (6)
O2—Mn2—O8—C24	−102.9 (4)	C15—C14—C23—C22	4.4 (9)
O3^{iii}—Mn2—O8—C24	−24.9 (8)	C13—C14—C23—C22	−178.9 (6)

O7—Mn2—O8—C24	−1.5 (4)	C21—C22—C23—C14	−3.4 (10)
N5—Mn2—O8—C24	155.2 (4)	Mn2—O8—C24—O7	2.6 (6)
N8—Mn2—O8—C24	81.7 (4)	Mn2—O8—C24—C21	−179.3 (6)
O4^{ii}—Mn1—N1—C25	−8.7 (6)	Mn2—O7—C24—O8	−2.9 (7)
O1^{i}—Mn1—N1—C25	89.0 (6)	Mn2—O7—C24—C21	179.0 (5)
O6—Mn1—N1—C25	−127.2 (6)	C22—C21—C24—O8	−146.0 (6)
N4—Mn1—N1—C25	179.5 (6)	C20—C21—C24—O8	34.0 (9)
O5—Mn1—N1—C25	−91.4 (6)	C22—C21—C24—O7	32.2 (9)
C13—Mn1—N1—C25	−102.6 (6)	C20—C21—C24—O7	−147.8 (6)
O4^{ii}—Mn1—N1—C29	173.2 (4)	C29—N1—C25—C26	−2.0 (10)
O1^{i}—Mn1—N1—C29	−89.1 (5)	Mn1—N1—C25—C26	179.9 (6)
O6—Mn1—N1—C29	54.7 (6)	N1—C25—C26—C27	1.7 (12)
N4—Mn1—N1—C29	1.4 (4)	C25—C26—C27—C28	0.0 (12)
O5—Mn1—N1—C29	90.5 (5)	C26—C27—C28—C29	−1.2 (11)
C13—Mn1—N1—C29	79.3 (5)	C26—C27—C28—C30	179.8 (7)
O1^{i}—Mn1—N4—C43	−77.6 (6)	C25—N1—C29—C28	0.7 (10)
O6—Mn1—N4—C43	24.5 (5)	Mn1—N1—C29—C28	178.9 (5)
N1—Mn1—N4—C43	180.0 (6)	C25—N1—C29—C40	−179.1 (6)
O5—Mn1—N4—C43	82.3 (5)	Mn1—N1—C29—C40	−0.8 (7)
C13—Mn1—N4—C43	53.1 (6)	C27—C28—C29—N1	0.9 (10)
O1^{i}—Mn1—N4—C40	100.5 (5)	C30—C28—C29—N1	180.0 (6)
O6—Mn1—N4—C40	−157.4 (5)	C27—C28—C29—C40	−179.4 (6)
N1—Mn1—N4—C40	−1.9 (4)	C30—C28—C29—C40	−0.3 (10)
O5—Mn1—N4—C40	−99.6 (5)	C31—N2—C30—C38	−0.3 (8)
C13—Mn1—N4—C40	−128.8 (5)	C31—N2—C30—C28	179.8 (7)
O2—Mn2—N5—C44	5.6 (7)	C29—C28—C30—C38	1.5 (10)
O3^{iii}—Mn2—N5—C44	−91.5 (6)	C27—C28—C30—C38	−179.5 (7)
O7—Mn2—N5—C44	122.3 (6)	C29—C28—C30—N2	−178.6 (7)
N8—Mn2—N5—C44	179.2 (7)	C27—C28—C30—N2	0.4 (12)
O8—Mn2—N5—C44	88.5 (6)	C30—N2—C31—N3	0.3 (8)
C24—Mn2—N5—C44	101.7 (6)	C30—N2—C31—C32	−176.1 (7)
O2—Mn2—N5—C48	−172.7 (5)	C38—N3—C31—N2	−0.1 (8)
O3^{iii}—Mn2—N5—C48	90.2 (5)	C38—N3—C31—C32	176.3 (7)
O7—Mn2—N5—C48	−56.0 (6)	N2—C31—C32—C37	172.2 (7)
N8—Mn2—N5—C48	0.9 (5)	N3—C31—C32—C37	−3.8 (11)
O8—Mn2—N5—C48	−89.9 (5)	N2—C31—C32—C33	−6.2 (11)
C24—Mn2—N5—C48	−76.7 (5)	N3—C31—C32—C33	177.8 (7)
O3^{iii}—Mn2—N8—C62	74.5 (6)	C37—C32—C33—C34	−1.3 (11)
O7—Mn2—N8—C62	−32.8 (6)	C31—C32—C33—C34	177.2 (7)
N5—Mn2—N8—C62	177.3 (7)	C32—C33—C34—C35	1.5 (13)
O8—Mn2—N8—C62	−89.5 (6)	C33—C34—C35—C36	−0.3 (13)
C24—Mn2—N8—C62	−61.4 (6)	C34—C35—C36—C37	−1.0 (12)
O3^{iii}—Mn2—N8—C59	−100.8 (5)	C35—C36—C37—C32	1.2 (12)
O7—Mn2—N8—C59	152.0 (5)	C33—C32—C37—C36	−0.1 (11)
N5—Mn2—N8—C59	2.0 (5)	C31—C32—C37—C36	−178.5 (7)
O8—Mn2—N8—C59	95.2 (5)	N2—C30—C38—N3	0.3 (8)
C24—Mn2—N8—C59	123.4 (5)	C28—C30—C38—N3	−179.8 (6)
C6—C1—C2—C3	0.0	N2—C30—C38—C39	179.0 (6)

C11—C1—C2—C3	−179.8 (9)	C28—C30—C38—C39	−1.1 (11)
C1—C2—C3—C4	0.0	C31—N3—C38—C30	−0.1 (7)
C2—C3—C4—C5	0.0	C31—N3—C38—C39	−178.7 (7)
C2—C3—C4—C12	−173.3 (9)	C30—C38—C39—C40	−0.7 (10)
C3—C4—C5—C6	0.0	N3—C38—C39—C40	177.7 (7)
C12—C4—C5—C6	172.9 (10)	C30—C38—C39—C41	−177.5 (7)
C3—C4—C5—C10	180.0	N3—C38—C39—C41	0.9 (12)
C12—C4—C5—C10	−7.1 (10)	C43—N4—C40—C39	1.2 (10)
C4—C5—C6—C7	180.0	Mn1—N4—C40—C39	−177.0 (5)
C10—C5—C6—C7	0.0	C43—N4—C40—C29	−179.6 (6)
C4—C5—C6—C1	0.0	Mn1—N4—C40—C29	2.2 (7)
C10—C5—C6—C1	180.0	C38—C39—C40—N4	−178.9 (6)
C2—C1—C6—C7	180.0	C41—C39—C40—N4	−1.8 (10)
C11—C1—C6—C7	−0.2 (9)	C38—C39—C40—C29	1.9 (9)
C2—C1—C6—C5	0.0	C41—C39—C40—C29	179.0 (6)
C11—C1—C6—C5	179.8 (9)	N1—C29—C40—N4	−1.0 (9)
C5—C6—C7—C8	0.0	C28—C29—C40—N4	179.3 (6)
C1—C6—C7—C8	180.0	N1—C29—C40—C39	178.2 (6)
C6—C7—C8—C9	0.0	C28—C29—C40—C39	−1.5 (10)
C7—C8—C9—C10	0.0	C40—C39—C41—C42	2.1 (10)
C8—C9—C10—C5	0.0	C38—C39—C41—C42	178.9 (7)
C6—C5—C10—C9	0.0	C39—C41—C42—C43	−1.9 (11)
C4—C5—C10—C9	180.0	C40—N4—C43—C42	−0.9 (10)
C6′—C1′—C2′—C3′	0.0	Mn1—N4—C43—C42	177.1 (5)
C11—C1′—C2′—C3′	176.5 (9)	C41—C42—C43—N4	1.3 (12)
C1′—C2′—C3′—C4′	0.0	C48—N5—C44—C45	0.8 (12)
C2′—C3′—C4′—C5′	0.0	Mn2—N5—C44—C45	−177.5 (7)
C2′—C3′—C4′—C12	−177.1 (8)	N5—C44—C45—C46	−2.2 (15)
C3′—C4′—C5′—C6′	0.0	C44—C45—C46—C47	1.9 (15)
C12—C4′—C5′—C6′	176.9 (8)	C45—C46—C47—C48	−0.5 (12)
C3′—C4′—C5′—C10′	180.0	C45—C46—C47—C49	−178.7 (8)
C12—C4′—C5′—C10′	−3.1 (8)	C44—N5—C48—C47	0.7 (10)
C4′—C5′—C6′—C7′	180.0	Mn2—N5—C48—C47	179.1 (5)
C10′—C5′—C6′—C7′	0.0	C44—N5—C48—C59	178.1 (6)
C4′—C5′—C6′—C1′	0.0	Mn2—N5—C48—C59	−3.4 (7)
C10′—C5′—C6′—C1′	180.0	C46—C47—C48—N5	−0.8 (11)
C2′—C1′—C6′—C7′	180.0	C49—C47—C48—N5	177.5 (6)
C11—C1′—C6′—C7′	3.6 (9)	C46—C47—C48—C59	−178.2 (7)
C2′—C1′—C6′—C5′	0.0	C49—C47—C48—C59	0.1 (10)
C11—C1′—C6′—C5′	−176.4 (9)	C50—N6—C49—C57	−0.9 (8)
C5′—C6′—C7′—C8′	0.0	C50—N6—C49—C47	−178.9 (7)
C1′—C6′—C7′—C8′	180.0	C48—C47—C49—N6	175.6 (7)
C6′—C7′—C8′—C9′	0.0	C46—C47—C49—N6	−6.2 (13)
C7′—C8′—C9′—C10′	0.0	C48—C47—C49—C57	−2.2 (10)
C8′—C9′—C10′—C5′	0.0	C46—C47—C49—C57	176.0 (7)
C4′—C5′—C10′—C9′	180.0	C49—N6—C50—N7	0.9 (8)
C6′—C5′—C10′—C9′	0.0	C49—N6—C50—C51	176.8 (7)
Mn2—O2—C11—O1	25.4 (13)	C57—N7—C50—N6	−0.6 (8)

Mn2—O2—C11—C1	−153.6 (6)	C57—N7—C50—C51	−176.5 (7)
Mn2—O2—C11—C1′	−158.4 (6)	N6—C50—C51—C52	5.0 (12)
Mn1^{v}—O1—C11—O2	−116.3 (8)	N7—C50—C51—C52	−179.6 (7)
Mn1^{v}—O1—C11—C1	62.7 (9)	N6—C50—C51—C56	−172.3 (7)
Mn1^{v}—O1—C11—C1′	67.7 (9)	N7—C50—C51—C56	3.1 (12)
C2—C1—C11—O2	−128.5 (7)	C56—C51—C52—C53	1.0 (14)
C6—C1—C11—O2	51.7 (11)	C50—C51—C52—C53	−176.3 (8)
C2—C1—C11—O1	52.5 (9)	C51—C52—C53—C54	−2.7 (16)
C6—C1—C11—O1	−127.3 (7)	C52—C53—C54—C55	1.8 (17)
C2—C1—C11—C1′	−66 (7)	C53—C54—C55—C56	0.7 (16)
C6—C1—C11—C1′	114 (7)	C52—C51—C56—C55	1.5 (13)
C2′—C1′—C11—O2	59.2 (9)	C50—C51—C56—C55	178.7 (8)
C6′—C1′—C11—O2	−124.4 (8)	C54—C55—C56—C51	−2.4 (14)
C2′—C1′—C11—O1	−124.4 (7)	C50—N7—C57—C49	0.0 (7)
C6′—C1′—C11—O1	52.0 (11)	C50—N7—C57—C58	176.6 (7)
C2′—C1′—C11—C1	−60 (7)	N6—C49—C57—N7	0.6 (8)
C6′—C1′—C11—C1	116 (7)	C47—C49—C57—N7	178.8 (6)
Mn1^{iv}—O4—C12—O3	−27.7 (11)	N6—C49—C57—C58	−176.3 (7)
Mn1^{iv}—O4—C12—C4′	148.4 (6)	C47—C49—C57—C58	1.9 (11)
Mn1^{iv}—O4—C12—C4	156.8 (6)	N7—C57—C58—C60	2.2 (13)
Mn2^{vi}—O3—C12—O4	114.4 (8)	C49—C57—C58—C60	178.2 (7)
Mn2^{vi}—O3—C12—C4′	−61.8 (8)	N7—C57—C58—C59	−175.3 (7)
Mn2^{vi}—O3—C12—C4	−70.3 (9)	C49—C57—C58—C59	0.7 (11)
C5′—C4′—C12—O4	−53.8 (10)	C62—N8—C59—C58	0.3 (10)
C3′—C4′—C12—O4	123.1 (6)	Mn2—N8—C59—C58	175.9 (5)
C5′—C4′—C12—O3	122.6 (7)	C62—N8—C59—C48	180.0 (6)
C3′—C4′—C12—O3	−60.4 (7)	Mn2—N8—C59—C48	−4.4 (8)
C5′—C4′—C12—C4	−121 (5)	C60—C58—C59—N8	−0.9 (11)
C3′—C4′—C12—C4	56 (4)	C57—C58—C59—N8	176.9 (6)
C3—C4—C12—O4	−58.9 (8)	C60—C58—C59—C48	179.5 (7)
C5—C4—C12—O4	128.0 (7)	C57—C58—C59—C48	−2.8 (10)
C3—C4—C12—O3	125.4 (6)	N5—C48—C59—N8	5.3 (9)
C5—C4—C12—O3	−47.7 (11)	C47—C48—C59—N8	−177.2 (6)
C3—C4—C12—C4′	58 (4)	N5—C48—C59—C58	−175.0 (6)
C5—C4—C12—C4′	−116 (5)	C47—C48—C59—C58	2.4 (10)
Mn1—O6—C13—O5	−3.8 (7)	C59—C58—C60—C61	1.3 (12)
Mn1—O6—C13—C14	179.5 (5)	C57—C58—C60—C61	−176.2 (8)
Mn1—O5—C13—O6	3.4 (6)	C58—C60—C61—C62	−1.2 (13)
Mn1—O5—C13—C14	−179.9 (5)	C59—N8—C62—C61	−0.2 (12)
O6—C13—C14—C23	151.0 (6)	Mn2—N8—C62—C61	−175.3 (6)
O5—C13—C14—C23	−25.9 (8)	C60—C61—C62—N8	0.6 (13)
O6—C13—C14—C15	−32.5 (9)	C64—N9—C63—O9	−0.3 (4)
O5—C13—C14—C15	150.6 (6)	C65—N9—C63—O9	−179.8 (13)
C23—C14—C15—C16	177.6 (6)		

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) *x*+1, *y*+1, *z*; (iii) *x*+1, *y*, *z*; (iv) *x*−1, *y*−1, *z*; (v) *x*, *y*−1, *z*; (vi) *x*−1, *y*, *z*.